

Limitations of spin-fermion models in studying underdoped cuprates

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A microscopic basis is provided for the spin-fermion model used to describe the physics of the underdoped cuprates. In this way, a spin-fermion coupling is shown to take care of the local no double occupancy constraint, which is ignored in the weakly coupled regime. This ingredient is proved to be essential to capture the physics of strong correlations, however. We elaborate further on our recent proposal for the strong-coupling version of the spin-fermion model that may prove to be the correct starting point to deal with the strong correlation physics displayed by the underdoped cuprates.

I. INTRODUCTION: SPIN-FERMION MODEL

The purpose of this work is to establish a reliable microscopic basis for the spin-fermion (SF) model which might be appropriate to describe the physics of the lightly doped cuprates. Since there are several different versions of the SF model in use to describe the high- T_c superconductors it is important to discuss initially how they differ from each other.

More than a decade ago the SF model was put forward in an attempt to account for the observed non-Fermi liquid anomalies in the doped cuprates near optimal doping.[1] This original model essentially describes low-energy fermions with a large Fermi surface (FS) interacting with each other via soft collective spin excitations,

$$\mathcal{L}_{sf} = \mathcal{L}_c + \mathcal{L}_\lambda + \mathcal{L}_\phi,$$

where

$$\begin{aligned} \mathcal{L}_c &= \sum_i c_{i\alpha}^\dagger (\partial_\tau - \mu) c_{i\alpha} - \sum_{i < j} t_{ij} (c_{i\alpha}^\dagger c_{j\alpha} + c_{j\alpha}^\dagger c_{i\alpha}), \\ \mathcal{L}_\lambda &= \lambda \sum_i \phi_i^a c_{i\alpha}^\dagger \sigma_{\alpha\beta}^a c_{i\beta}, \\ \mathcal{L}_\phi &= \sum_q \chi_0^{-1} \vec{\phi}_q \vec{\phi}_{-\vec{q}}. \end{aligned} \quad (1)$$

Here $c_{i\alpha}^\dagger$ is the creation operator for electrons with spin projection $\alpha = \uparrow, \downarrow$ on site i , the amplitudes t_{ij} are hopping matrix elements describing the "large" Fermi surface, μ is a chemical potential, and σ^a , $a = x, y, z$, are the Pauli matrices.

The bare spin propagator emerges from the integration of the high-energy fermionic modes,

$$\chi_0(q = \vec{q}, \omega_n) = \left(\frac{\omega_n^2}{v_s^2} + (\vec{q} - \vec{Q})^2 + \xi_{AF}^{-2} \right)^{-1}, \quad (2)$$

where $\omega_n = 2\pi n/\beta$ are Matsubara bosonic frequencies. The antiferromagnetic (AF) spin correlation length, ξ_{AF} , and the spin velocity v_s are high-energy phenomenological parameters. At criticality ($\xi_{AF} = \infty$), the singular

nature of the low-energy AF paramagnons singles out the so-called *hotspots* on the FS connected by \vec{Q} . Those points are precisely the intersects of the large hole-like FS with the magnetic zone boundary.

Due to the enormous enhancement of the AF fluctuations at or near the quantum critical point (QCP), the fermions in the vicinity of the hotspots interact strongly with each other via singular AF paramagnons. This results in strong damping of the propagating spin modes. The spin modes become dissipative and the fermions quasiparticles acquire a short lifetime. As a result, the electron system displays a singular non-FL infrared behaviour declared to be observed in the cuprates near optimal doping.[1] In principle, the SF model is a FL theory plagued with infrared singularities in an attempt to account for a non-FL low-energy physics of the optimally doped cuprates.

This SF model can be formally derived from the Hubbard model [1] which describes fermions hopping on a lattice with a tunneling amplitude t_{ij} and are subjected to a short-range Coulomb repulsion U ,

$$H_U = - \sum_{i,j} t_{ij\alpha} (c_{i\alpha}^\dagger c_{j\alpha} - \mu) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (3)$$

where $n_{i\alpha} = c_{i\alpha}^\dagger c_{i\alpha}$ is the on-site electron number operator. Following standard procedure the quartic fermion interaction can be decoupled using a Hubbard-Stratonovich field $\vec{\phi}$ that physically corresponds to the collective spin excitations which are "made out" of the fermion degrees of freedom. This procedure can be justified only if the SF coupling $\lambda \sim U$ is smaller than the fermionic bandwidth $W \sim t$, where t is a nearest-neighbour hopping amplitude. This automatically brings the theory into a weak-coupling regime controlled by a small parameter, U/t .

The requirement $U/t \ll 1$ implies that strong electron correlations due a large on-site Coulomb repulsion U are totally ignored. This may correspond to an overdoped region of the cuprate phase diagram that displays a conventional FL physics. With some modifications (the hot spots theory, etc.) being imposed, it exhibits a non-FL behaviour that might be thought of as being relevant

to the optimally doped cuprates, provided the strange metal phase has nothing to do with strong correlations. However, this approach is inapplicable to lower dopings in which strong correlations are known to be at work. In particular, the underdoped pseudogap (PG) region is characterized by strong electron correlations which keep the majority of the electrons well localized. Accordingly, the FS consists of small separated patches (electron pockets) as observed in the quantum-oscillation experiments.

The observation of quantum oscillations in the lightly hole-doped cuprates is an important breakthrough since it indicates that coherent electronic quasiparticles may exist even in the PG regime. The PG state does not exhibit a large FS enclosing a total number of charged carriers. Instead the FS consists of small pockets with a total area proportional to a dopant density x , rather than $1+x$ which is expected for conventional FL's. There are two routes to a Fermi surface reconstruction that could apply to the cuprates. A possible theoretical justification for this phenomenon might be the occurrence of a simultaneous setting of a new long-range order together with the PG phase at a critical hole concentration, $x_c \approx 0.19$. The resulting breakdown of translational symmetry would cut the large FS into small pieces but the Luttinger's theorem (LT) would still hold. This is exactly what the conventional SF model predicts. However, so far there are no observations of the existence of any order parameter that breaks translation symmetry near $x = x_c$.

II. FRACTIONALIZED FERMI-LIQUID MODEL

The fractionalized Fermi-liquid (FL*) was proposed phenomenologically as an alternative to describe lightly doped antiferromagnets. It goes beyond the weak coupling regime and as a result it is able to produce small Fermi pockets without translational symmetry breaking. The Lagrangian density of this new model is [2]

$$\begin{aligned}\mathcal{L}'_{sf} &= \mathcal{L}'_c + \mathcal{L}'_\lambda + \mathcal{L}'_n, \\ \mathcal{L}'_c &= \sum_i c_{i\alpha}^\dagger (\partial_\tau - \mu) c_{i\alpha} - \sum_{i < j} t_{ij} (c_{i\alpha}^\dagger c_{j\alpha} + c_{j\alpha}^\dagger c_{i\alpha}), \\ \mathcal{L}'_\lambda &= \lambda \sum_i (-1)^{x_i + y_i} n_i^a c_{i\alpha}^\dagger \sigma_{\alpha\beta}^a c_{i\beta}, \\ \mathcal{L}'_n &= \frac{1}{2g} \int d^2r [(\partial_\tau n^a)^2 + v_s^2 (\partial_r n^a)^2].\end{aligned}\quad (4)$$

Three phenomenological parameters enter into Eq.(4): the parameter λ represents a spin-fermion coupling, g controls the strength of the antiferromagnetic (AF) fluctuations, and v_s stands for the spin velocity.

There are two basic distinctions between the conventional SF model [1] and that given by (4). i) The conventional SF model is controlled by a small parameter

$\lambda/t \ll 1$. Only under this condition, can the SF model be justified as a low-energy approximation to the Hubbard model. The physical meaning of the coupling λ in the conventional approach is that it represents a spin density wave (SDW) gap. In contrast, in Eq.(4), λ should be considered as a coupling of order t and it has nothing to do with the SDW gap.

ii) The spin sector in the conventional SF model is described by a soft spin mode $\vec{\phi}$ which appears as a Hubbard-Stratonovich auxiliary field to linearize the quartic fermion coupling. This mode is "made out" of the fermionic degrees of freedom which necessarily implies that the spin velocity v_s is of order the relevant Fermi velocity, $v_s \sim v_F \sim ta$, with a being the lattice spacing. In contrast, in the model (4), the spin sector is described instead by the "hard-spin" field n^a that obeys the local constraint $\sum_a (n^a)^2 = 1$. The spin-1 order parameter \vec{n} can be split into two spin-1/2 charge neutral spinons z_α :

$$n^a = \bar{z}_{i\alpha} \sigma_{\alpha\beta}^a z_{i\beta}, \quad \bar{z}_{i\alpha} z_{i\alpha} = 1.$$

The emergent gauge field, $z_{i\alpha} \rightarrow z_{i\alpha} e^{i\theta_i}$, glues them together.

The compact $U(1)$ gauge theory is at strong coupling (there is no Maxwell term in the action) and it is presumably in a confining phase. If one assumes however that there exists an energy window in which the deconfinement does indeed take place, one can derive the small-pocket FS within an effective FL* theory based on the spinon decomposition of the order parameter and on symmetry considerations.[2] It is not totally clear what controls such a theory, however. For instance, the key equation (3.1) in [2] rewrites the conventional electron on-site operator c_α in terms of a new (unitary equivalent) $SU(2)$ spinor ψ_\pm :

$$c_\alpha = z_\alpha \psi_+ - \epsilon_{\alpha\beta} \bar{z}_\beta \psi_- \approx Z(F_\alpha + G_\alpha), \quad (5)$$

where Z is some constant factor, $\epsilon_{\alpha\beta}$ is a totally antisymmetric tensor, $\epsilon_{\uparrow\downarrow} = 1$, and z_α a set of complex numbers subject to the condition $\sum_\alpha \bar{z}_\alpha z_\alpha = 1$. Although the electron operator c_α by definition transforms itself as an $SU(2)$ spinor, the $z_\alpha \psi_+$ and $\epsilon_{\alpha\beta} \bar{z}_\beta \psi_-$ operators taken apart from each other do not transform in the same way. Nevertheless, a true single fermion operator splits into a sum of two *independent* fermion modes, F_α and G_α . It is not obvious what controls the approximation made in Eq.(5).

On the other hand, when an emergent gauge field is indeed in the deconfined phase (e.g., \mathcal{Z}_2 gauge field in $2+1$) the spinons can appear in the physical spectrum. To get the gauge field deconfined one needs first to have it gapped. This is a necessary condition to arrive at the FL* phase. One route to achieve this is to apply a MF theory that breaks $U(1)$ down to \mathcal{Z}_2 [3]. However, such a theory can be controlled only in the limit where the

spin exchange term is much larger than the hopping term which is not the case for the cuprates, however.

An alternative approach was recently proposed in [4]. Roughly speaking it involves a direct coupling of a spinon field in the phenomenological SF model (4) to a \mathbb{Z}_2 gauge field. A crucial requirement in this approach is that the coupling λ is to be considered as the largest energy scale in the problem. The topological order and fractionalization appear in a regime inaccessible in a small λ expansion.

III. ITINERANT-LOCALIZED MODEL OF STRONG CORRELATIONS

In the present paper we show that the starting point employed in [2] – the phenomenological SF model (4) – can in fact be derived microscopically up to a certain λ -dependent extra term by employing the earlier established mapping of the $t - J$ model of strongly correlated electrons onto the Kondo-Heisenberg model at a dominantly large Kondo coupling [5]. This enable us to clarify the physical meaning of the coupling λ in (4) and, in this way, to understand the possible physical limitations of the SF models in describing the physics of the underdoped cuprates.

Let us start with the observation that, in the underdoped cuprates, one striking feature is the simultaneous existence of both localized and itinerant nature of the lattice electrons. To include both aspects into consideration on equal footing, Ribeiro and Wen proposed a slave-particle spin-dopon representation of the projected electron operators in the enlarged Hilbert space [6],

$$\tilde{c}_i^\dagger = c_i^\dagger(1 - n_{i-\sigma}) = \frac{1}{\sqrt{2}}\left(\frac{1}{2} - 2\vec{S}_i \cdot \vec{\sigma}\right)\tilde{d}_i. \quad (6)$$

In this framework, the localized electron is represented by the lattice spin $\vec{S} \in su(2)$ whereas the doped hole (dopon) is described by the projected hole operator, $\tilde{d}_{i\alpha} = d_{i\sigma}(1 - n_{i-\alpha}^d)$. Here $\tilde{c}^\dagger = (\tilde{c}_\uparrow^\dagger, \tilde{c}_\downarrow^\dagger)^t$ and $\tilde{d} = (\tilde{d}_\uparrow, \tilde{d}_\downarrow)^t$.

In terms of the projected electron operators, the constraint of no double occupancy (NDO) takes on the form

$$\sum_{\alpha} (\tilde{c}_{i\alpha}^\dagger \tilde{c}_{i\alpha}) + \tilde{c}_{i\alpha} \tilde{c}_{i\alpha}^\dagger = 1. \quad (7)$$

It singles out the physical $3d$ on-site Hilbert space. Only under this condition are the projected electron operators isomorphic to the original Hubbard operators. Within the spin-dopon representation, the NDO constraint reduces to a Kondo-type interaction,[5]

$$\vec{S}_i \cdot \vec{s}_i + \frac{3}{4}(\tilde{d}_{i\uparrow}^\dagger \tilde{d}_{i\uparrow} + \tilde{d}_{i\downarrow}^\dagger \tilde{d}_{i\downarrow}) = 0, \quad (8)$$

with $\vec{s}_i = \sum_{\alpha,\beta} \tilde{d}_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \tilde{d}_{i\beta}$ being the dopon spin operator.

Proceeding with Eq.(8) we end up with the lattice Kondo-Heisenberg model which, at strong coupling ($\lambda \gg t$), is equivalent to the original $t - J$ model:

$$H_{t-J} = \sum_{ij\sigma} 2t_{ij} d_{i\sigma}^\dagger d_{j\sigma} + J \sum_{ij} \vec{S}_i(1 - n_i^d) \cdot \vec{S}_j(1 - n_j^d) + \lambda \sum_i (\vec{S}_i \cdot \vec{s}_i + \frac{3}{4}n_i^d), \quad \lambda \rightarrow +\infty. \quad (9)$$

In spite of the global character of the parameter λ , it enforces the NDO constraint locally due to the fact that the on-site physical Hilbert subspace corresponds to zero eigenvalues of the constraint, whereas the nonphysical subspace is spanned by the eigenvectors with strictly positive eigenvalues. As we showed elsewhere, in $1d$, Eq. (9) reproduces the well-known exact results for the $t - J$ model.[7]

The unphysical doubly occupied electron states are separated from the physical sector by an energy gap $\sim \lambda$. In the $\lambda \rightarrow +\infty$ limit, i.e. in the limit in which λ is much larger than any other existing energy scale in the problem, those states are automatically excluded from the Hilbert space. On the other hand, in this limit, the high and low energy itinerant fermions cannot be separated out and this is another manifestation of the local Mott physics. In view of that it does not seem appropriate to integrate out the high-energy fermions. We assume however that this separation still holds in the spin-dopon representation for well localized particles, i.e., the localized spin degrees of freedom. In this way we arrive [8] at an effective Lagrangian to describe strongly correlated electrons in the underdoped phase:

$$\begin{aligned} \tilde{\mathcal{L}} &= \tilde{\mathcal{L}}_d + \tilde{\mathcal{L}}_\lambda + \tilde{\mathcal{L}}_n, \\ \tilde{\mathcal{L}}_d &= \sum_i d_{i\alpha}^\dagger (\partial_\tau + \frac{3\lambda}{4} - \mu) d_{i\alpha} \\ &\quad + 2 \sum_{i < j} t_{ij} (d_{i\alpha}^\dagger d_{j\alpha} + d_{j\alpha}^\dagger d_{i\alpha}), \\ \tilde{\mathcal{L}}_\lambda &= \lambda \sum_i (-1)^{x_i+y_i} n_i^a d_{i\alpha}^\dagger \sigma_{\alpha\beta}^a d_{i\beta}, \\ \tilde{\mathcal{L}}_n &= \frac{1}{2g} \int d^2\vec{r} [(\partial_\tau n^a)^2 + v_s^2 (\partial_{\vec{r}} n^a)^2]. \end{aligned} \quad (10)$$

where $v_s = Ja$ is the spin-wave velocity, and $g = 4Ja^2/s$. In this model, the itinerant degrees of freedom are described by the dopons whereas the localized ones – by the fluctuating AF order parameter, n^a . In the limit $\lambda \rightarrow \infty$, the dopons and the lattice spins merge into the gauge neutral objects (6) to represent the physical electrons.

There are a few distinctions between \mathcal{L}' and $\tilde{\mathcal{L}}$. To start with, the model $\tilde{\mathcal{L}}$ is formulated in terms of the hole (dopon) operators d 's, rather than the electron operators c 's. It might seem, at first sight, that the electron-like

pockets should emerge in place of the hole-like pockets. However, this is not the case, since in our model the fermion dispersion changes sign, $t_{ij} \rightarrow -t_{ij}$. Note also that the renormalized hopping amplitude in $\tilde{\mathcal{L}}$ contains the spin-fermion coupling λ , as given by Eq.(10). Because of this, in the physical limit, $\lambda \rightarrow +\infty$, the model remains well defined and finite. Finally, the hopping amplitude in $\tilde{\mathcal{L}}$ contains an important factor of 2 that reflects the fact that a vacancy is now represented as a spin-dopon singlet (see, [5]).

The physical meaning of the Kondo coupling λ is that it takes care of the NDO constraint. As the quantum Monte Carlo simulations of the model (9) explicitly show [9], the NDO constraint plays the dominating role in the destruction of the long-range AF state. The critical hole concentration is around $x_c = 0.05$ at $J = 0.2t$. The spin-spin correlation functions at fixed doping become almost identical to each other for $\lambda \geq 10t$. This indicates that, in principle, finite but large enough values of λ already provide a reliable description of the existing strong correlations in the underdoped regime.

IV. FURTHER COMPARISONS OF THE MODELS

With this understanding of the physical meaning of the Kondo coupling λ , let us compare the \mathcal{L} and \mathcal{L}' SF models against the itinerant-localized $\tilde{\mathcal{L}}$ model. As the conventional SF model (1) implies $\lambda/t \ll 1$, it does not capture strong correlations at all. Its phenomenological modification given by (4) implies that $\lambda \sim t$. This might correspond to an optimally doped phase, provided the extra λ -term in the hopping term is also taken into account. In fact, its magnitude is of the same order as that of the t -term. In the \mathcal{Z}_2 gauge theory based on \mathcal{L}' and described in detail in [4], the crucial statement is that the λ is the largest energy scale. This, by definition, implies that the theory must remain finite and well defined at $\lambda = +\infty$, which physically corresponds to a regime of strong electron correlations.

There is an analogy with that and the conventional large U approximation to the Hubbard model referred to as the $t - J$ model. Namely, the Hubbard model reduces at $U = \infty$ to a well defined model that describes the so-called Nagaoka phase of strongly correlated electrons. The ground-state energy is finite and independent of U in the large- U limit. In contrast, the states obtained in [4] in the leading in λ approximation do not exhibit such a behaviour. For example, the ground state of the Mott insulator ($x = 0$) reads $E_G = -\lambda + \Delta - \mu$. The energy of the spinon excitation above the Mott insulator state takes the form $E_s = -\mu + 2\Delta - \sqrt{\lambda^2 + 4\Delta^2}$. Here μ and Δ are certain asymptotically λ -independent parameters. In particular, the FL* state is favoured in the limit $\lambda \gg \Delta \gg |t| \gg |J|$. [4] This implies that the

Mott insulator is not a stable phase in the physically well defined regime of strong electron correlations in which λ becomes boundless. This is hardly appropriate since those correlations are in fact a key ingredient behind the Mott physics.

On the other hand, if we follow all the steps exposed in [4] to compute those quantities starting right from the itinerant-localized model (10) we will obtain instead $E_G = \Delta - \mu$ and $E_s = -\mu + \lambda/2 + 2\Delta - \sqrt{\lambda^2/4 + 4\Delta^2}$. Both expressions remain finite, in the large λ limit. This occurs due to the fact that model (10) involves the extra λ -dependent renormalization of the hopping term which is missed in both \mathcal{L} and \mathcal{L}' SF models.

V. CONCLUSION

To conclude, we show that a number of unsatisfactory points that arise in an attempt to apply the SF-like models to treat the underdoped cuprates can be safely removed provided the itinerant-localized model of strongly correlated electrons is employed in their place. This indicates that this model may be the correct starting point to deal with the strong correlation physics displayed by the underdoped cuprates. Within a framework of the quantum Monte Carlo simulations, this model has recently been shown to provide a few interesting new results. In particular, the strong electron correlations are shown to play a key role in the abrupt destruction of the quasi-long-range AF order in the lightly doped regime.[9] This model was also employed to study the Nagaoka ($U = \infty$) limit of the Hubbard model to demonstrate the absence of the long-range ferromagnetic ordering at finite doping. [10]

A further possible application of the itinerant-localized model might be to theoretically explore an experimentally observed instability towards a d-wave formation of a charge order in the PG phase. This charge order seems to compete directly with the d-wave superconducting regime. There is a strong evidence that the observed charge order is due to strong electron correlations. This work is already in progress and results will be presented elsewhere.

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